

4,4'-(Propane-2,2-diyl)di(¹³C₆)phenol
263261-65-0 | DTXSID10675703

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 528 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.38e-01

Confidence level: 5.28e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl 1-naphthaleneacetate</div> <div>Measured: 302</div> <div>Predicted: 425</div>	<div>Image not found</div> <div>Isopropylpropyzamide</div> <div>Measured: 148</div> <div>Predicted: 173</div>	<div>Image not found</div> <div>3,3'-Dichlorobenzidine</div> <div>Measured: 22400</div> <div>Predicted: 1680</div>
<div>Image not found</div> <div>Siduron</div> <div>Measured: 204</div> <div>Predicted: 210</div>	<div>Image not found</div> <div>N-Cycloheptyl-N'-phenylurea</div> <div>Measured: 234</div> <div>Predicted: 218</div>	